Linking optical potentials to resonances at lower energies

Checking the accuracy of common approximations

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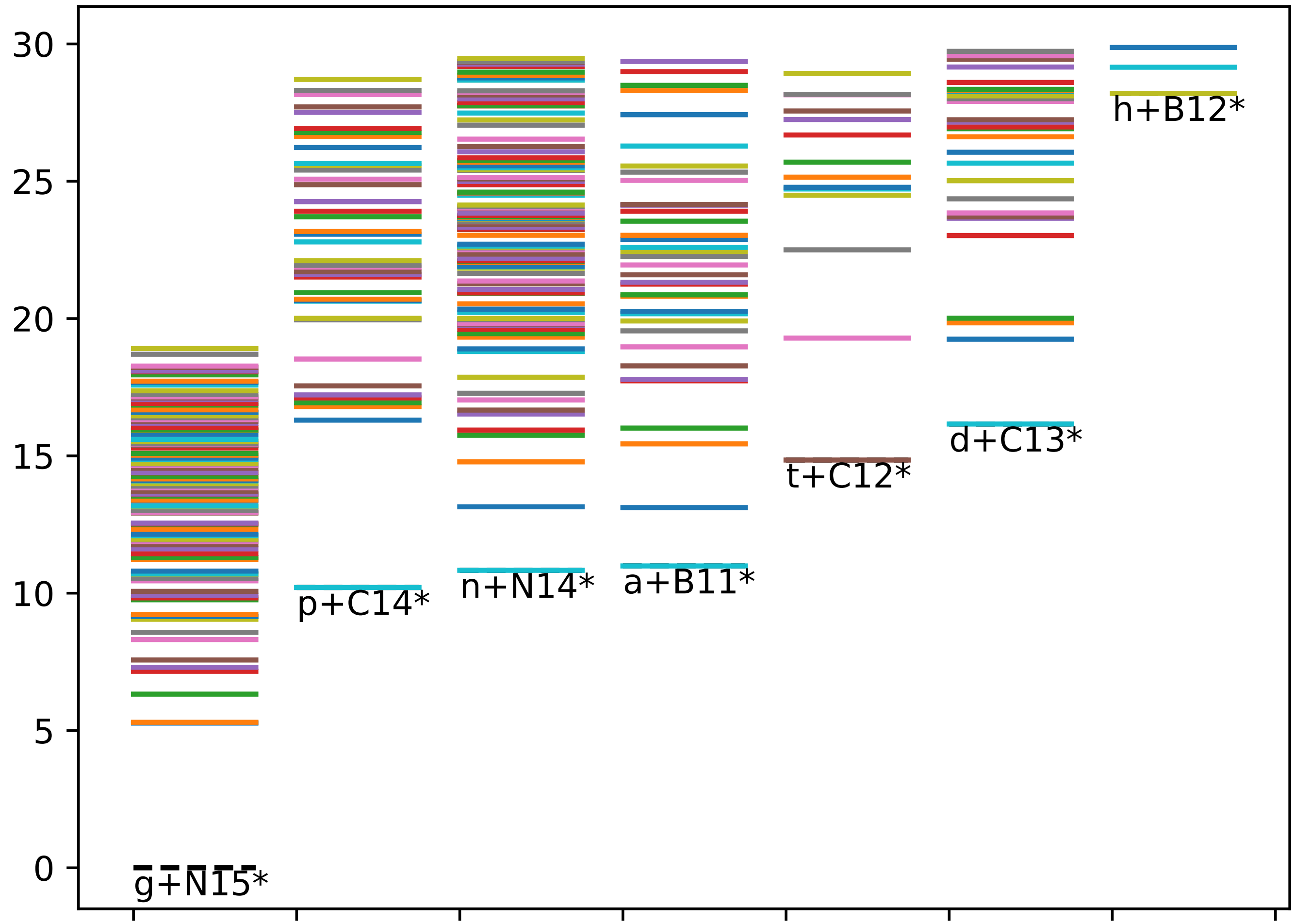
Summary

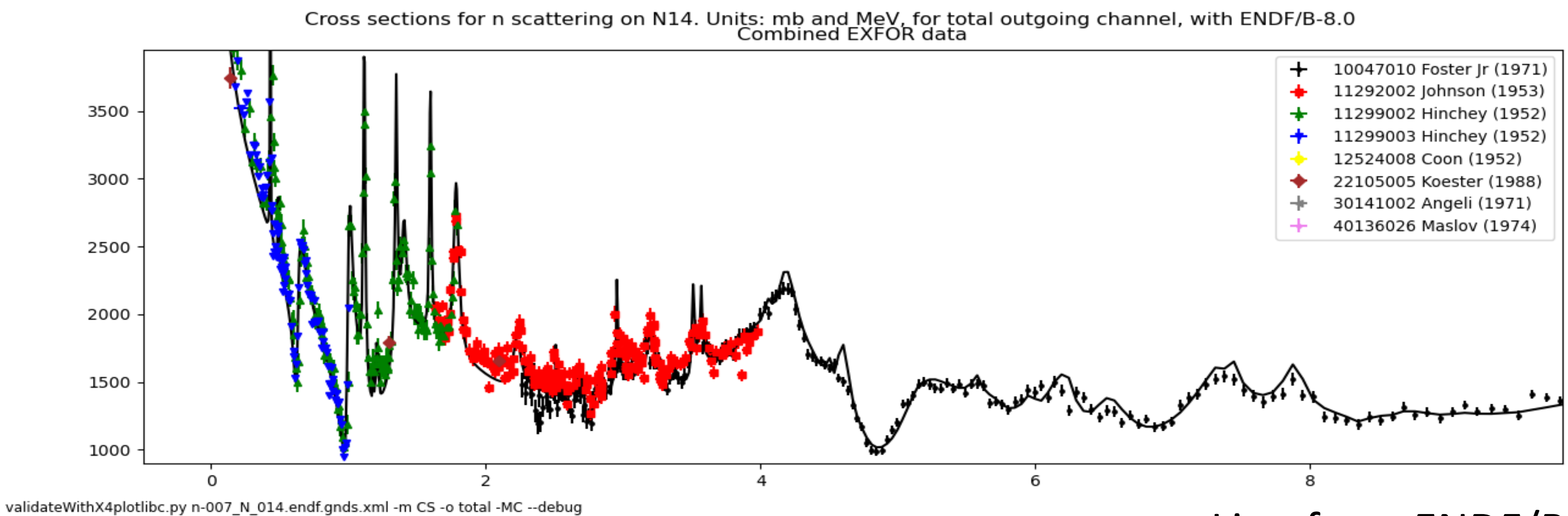
- Neutrons + ^{14}N reactions as a test case
- Known levels and level densities
- Going from R-matrix theory to Hauser-Feshbach models
- How to check the approximation used
- Try making R-matrix parameters to reproduce optical results, at least in middle range when resonances overlap more.

Known levels in n+N14 = N15* reactions

- Known levels from RIPL3:
- $^{15}N^*$ levels for incident neutrons
- n, p and α channels near.
- Many gamma decays from excited states.
- Needs a new evaluation!



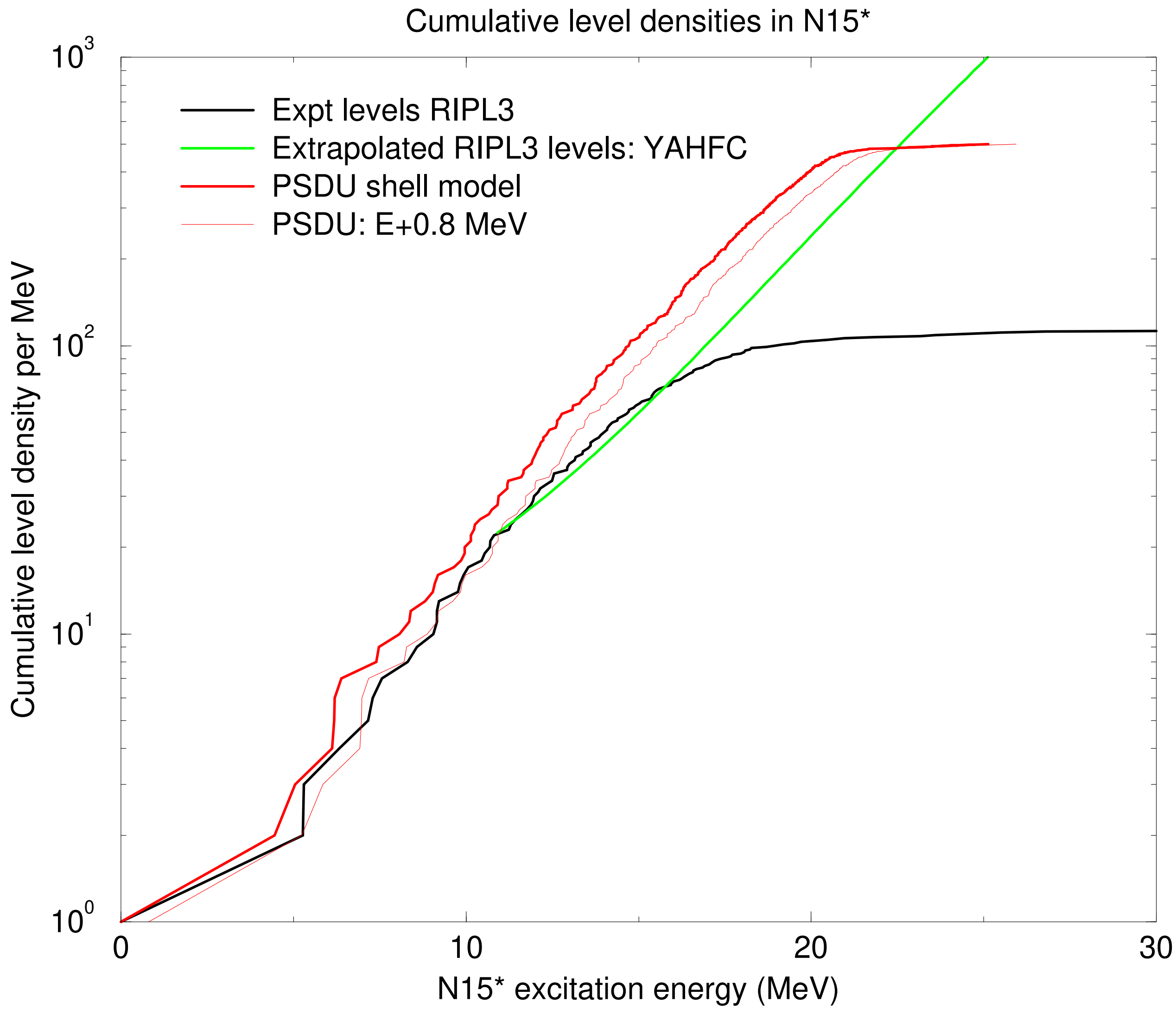
Neutron 'total cross-section' data from EXFOR



Line from ENDF/B-VIII.0

- Pronounced resonances < 4 MeV.
- Smoother > 4 MeV: unresolved resonances with higher densities
- Cannot search to fit individual resonances to this data > 4 MeV.

Level Densities: levels per MeV



RIPL3 levels for N15* as on level diagram.

R-matrix parameters

1. Diagonalize Hamiltonian inside R-matrix radius a
   – (with fixed ψ/ψ' to make orthonormal basis).
2. Energy eigenvalues ε_p for level p.
3. eigenstate wave functions $\psi_{p\alpha}(r)$
4. Wf values at $r = a$: $\gamma_{pa} = \sqrt{\frac{\hbar^2}{2\mu_\alpha a}}\psi_{pa}(a)$
   – Called 'reduced width amplitudes'
5. Formal width $\Gamma_{pa} = 2\,\gamma_{pa}^2 P_\alpha$. Penetrability $P_\alpha = \mathcal{I}m\,(\frac{aH^{+'}}{H^+})$
6. Total width $\Gamma_p = \sum_\alpha \Gamma_{pa}$

Exact R-matrix theory

For each specific spin and parity J^{π}_{tot}, the multichannel R matrix with N poles and channels α is

$$\mathbf{R}_{\alpha\alpha'}(E) = \sum_{p=1}^{N} \frac{\gamma_{p\alpha}\gamma_{p\alpha'}}{e_p - E}. \tag{1}$$

Using shift functions S and penetrability P, define shift and width matrices

$$\hat{\Delta}_{pq} + \tfrac{\mathrm{i}}{2}\hat{\Gamma}_{pq} = \sum_{\alpha} \gamma_{p\alpha}[S_\alpha + \mathrm{i}P_\alpha]\gamma_{q\alpha} \tag{2}$$

Construct the symmetric level matrix **A** is

$$(\mathbf{A}^{-1})_{pq} \quad = \quad \delta_{pq}(e_p - E) - \hat{\Delta}_{pq} - \tfrac{\mathrm{i}}{2}\hat{\Gamma}_{pq} \ , \tag{3}$$

that is

$$\mathbf{A} = -\begin{pmatrix} E - e_1 + \hat{\Delta}_{11} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{11} & \hat{\Delta}_{12} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{12} & \dots \\ \hat{\Delta}_{21} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{21} & E - e_2 + \hat{\Delta}_{22} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{22} & \dots \\ \dots & & \end{pmatrix}^{-1}, \tag{4}$$

The exact multi-channel multi-level $\tilde{\mathbf{S}}$ matrix is

$$\tilde{\mathbf{S}}_{\alpha'\alpha} = \Omega_\alpha \left[\delta_{\alpha'\alpha} + \mathrm{i} \sum_{\lambda\lambda'} \Gamma^{1/2}_{\alpha\lambda} \mathbf{A}_{\lambda\lambda'} \Gamma^{1/2}_{\alpha'\lambda'} \right] \Omega_{\alpha'}. \tag{5}$$

Single-level Breit-Wigner approximation (SLBW)

Neglect the off-diagonal terms of $\hat{\Gamma}_{pq}$ for *all* level interference terms:

$$\mathbf{A}_{pq} = \delta_{pq} \frac{1}{e_p - E - \hat{\Delta}_{pp} - \frac{\mathrm{i}}{2}\hat{\Gamma}_{pp}}, \tag{6}$$

from which the angle-integrated cross section to channel α' from α is

$$\sigma_{\alpha'\alpha}(J^{\pi}_{\text{tot}}; E) = \frac{\pi}{k^2}\, g_{J_{\text{tot}}} \sum_p \frac{\Gamma_{\alpha p}\Gamma_{\alpha' p}}{(E - E_p)^2 + \Gamma_p^2/4} \tag{7}$$

for spin coefficient $g_{J_{\text{tot}}}$. Each level p has a total width of $\Gamma_p = \sum_\alpha \Gamma_{\alpha p}$. The p-averaged cross section for average level spacing D is

$$\langle \sigma_{\alpha'\alpha}(E) \rangle = \frac{\pi}{k^2}\, g_{J_{\text{tot}}} \left\langle \frac{\Gamma_{\alpha p}\Gamma_{\alpha' p}}{\Gamma_p} \right\rangle \frac{2\pi}{D} \sim \frac{\pi}{k^2}\, g_{J_{\text{tot}}} \frac{\langle \Gamma_\alpha \rangle \langle \Gamma_{\alpha'} \rangle}{\langle \Gamma \rangle} \frac{2\pi}{D} \tag{8}$$

where the average sum $\langle \Gamma \rangle = \sum_\alpha \langle \Gamma_\alpha \rangle$.

The reaction cross-section: sum of all outgoing channels: $\sigma_R = \sum_{\alpha'} \sigma_{\alpha'\alpha}(E)$.

Connecting widths with optical potentials

The reaction cross-section from Eq. (8), the sum of all outgoing channels, is

$$\sigma_R = \frac{\pi}{k^2} g_{J_{\text{tot}}} \frac{2\pi\langle\Gamma_\alpha\rangle}{D} \tag{9}$$

This reaction cross section should equal the reaction cross section σ_R given by a one-channel optical potential and its S-matrix elements,

$$\sigma_R = \frac{\pi}{k_i^2} g_{J_{\text{tot}}} (1 - |\mathbf{S}_{\alpha_i\alpha_i}^{J_{\text{tot}}\pi}|^2) \tag{10}$$

arising from the flux leaving an entrance channel α_i.

Comparison of two expressions (9) and (10) gives

$$1 - |\mathbf{S}_{\alpha\alpha}^{\text{opt}}|^2 = \frac{2\pi\langle\Gamma_\alpha\rangle}{D} \quad \text{so} \quad \langle\Gamma_\alpha\rangle = \frac{D}{2\pi}(1 - |\mathbf{S}_{\alpha\alpha}^{\text{opt}}|^2). \tag{11}$$

Alternative expression (Simonius, 1974) giving larger widths when $|\mathbf{S}| \ll 1$:

$$\langle\Gamma_\alpha\rangle = -\frac{D}{2\pi} \ln(|\mathbf{S}_{\alpha\alpha}^{\text{opt}}|^2), \tag{12}$$

Checking the approximation used

1. The Single-level Breit-Wigner approximation
   a) Check effects of off-diagonal terms
   b) Check neglect of interferences for diagonal terms

2. Check that the width-fluctuation correction $W_{\alpha\alpha'}$ is near 1 in

$$\left\langle \frac{\Gamma_{\alpha p}\Gamma_{\alpha' p}}{\Gamma_p} \right\rangle = W_{\alpha\alpha'} \frac{\langle\Gamma_\alpha\rangle\langle\Gamma_{\alpha'}\rangle}{\langle\Gamma\rangle}$$

3. Check conversion from optical $|S_\alpha|^2$ to transmission coef T_α

4. Check overall Hauser-Feshbach models give cross-sections close to those from R-matrix models,
   at least in some transition region when both should work ok.

First: Compare R-matrix with HF cross-sections

- Use a range of known levels from RIPL3
  - Total cross-section has many resonances.
- Preliminary R-matrix fit to make plausible distributions.
- Use Koning-DelaRoche global optical potential for n+^{14}N
- Use YAHFC Hauser-Feshbach code to also predict cross-sections
- Compare:
  - Total cross-sections for neutrons: reaction + elastic
  - Transfer cross-sections to α + ^{11}B
  - Transfers to excited state (measured by their gamma decays)

Hauser-Feshbach models

The reaction cross-section from Eq. (8), the sum of all outgoing channels, is

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arising from the flux leaving an entrance channel α_i.

Comparison of two expressions (9) and (10) gives

$$1 - |\mathbf{S}^{\rm opt}_{\alpha\alpha}|^2 = \frac{2\pi\langle\Gamma_\alpha\rangle}{D}. \tag{11}$$

So we calculate *transmission coefficients* as

$$\mathcal{T}_\alpha = 1 - |\mathbf{S}^{\rm opt}_{\alpha\alpha}|^2, \tag{12}$$

in terms of which the channel cross sections of Eq. (8) become

$$\langle\sigma_{\alpha'\alpha}(J^\pi_{\rm tot}; E)\rangle = \frac{\pi}{k^2}\, g_{J_{\rm tot}} \frac{\mathcal{T}_\alpha \mathcal{T}_{\alpha'}}{\sum_{\alpha''}\mathcal{T}_{\alpha''}}. \tag{13}$$

The *Hauser-Feshbach branching ratios* here are

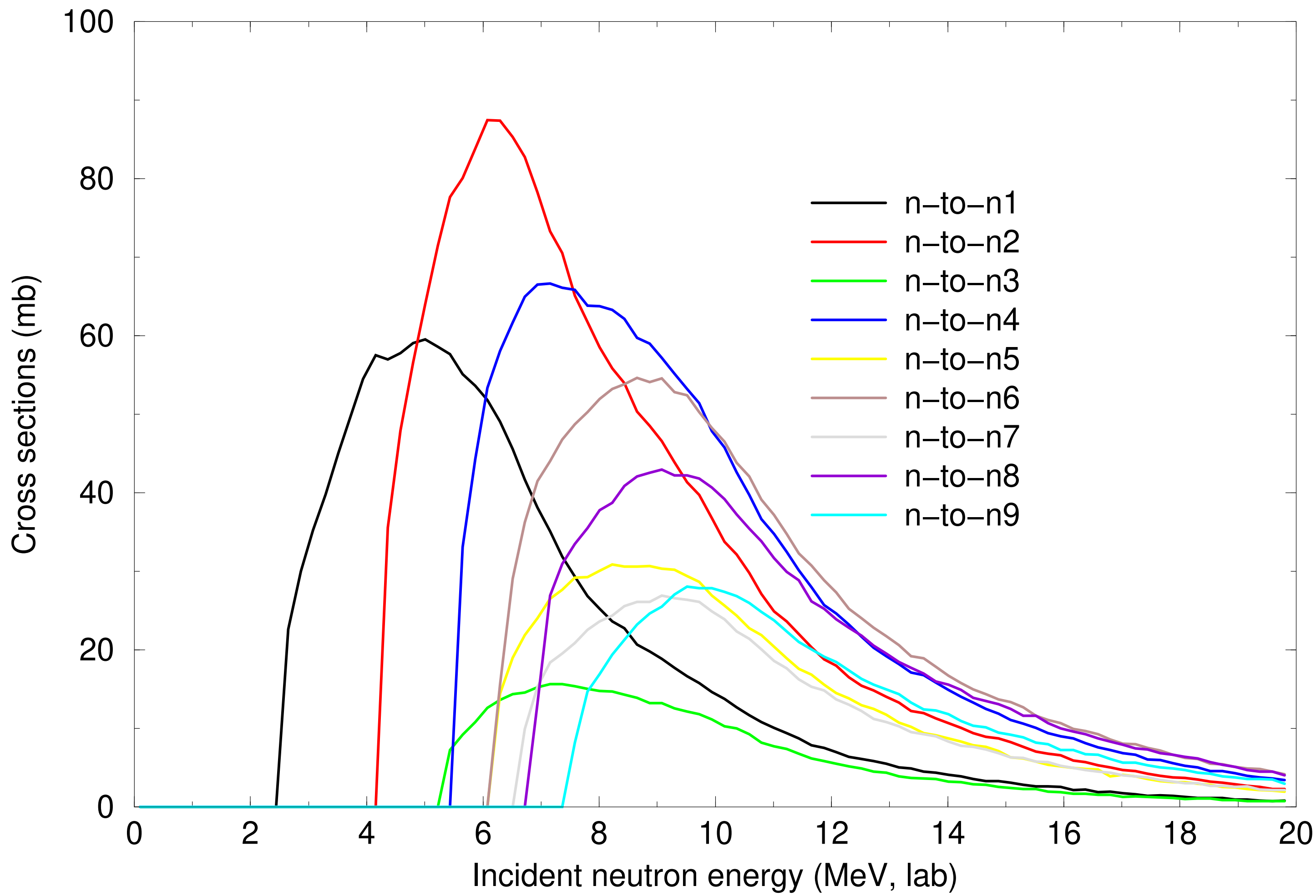
$$\mathcal{B}_{\alpha'} = \frac{\mathcal{T}_{\alpha'}}{\sum_{\alpha''}\mathcal{T}_{\alpha''}}. \tag{14}$$

Hauser-Feshbach cross-sections (smooth!)

Inelastic (n,n')

At higher energies even more inelastic channels.

Fusion neutrons at 14 MeV will require all these inelastic channels and more !



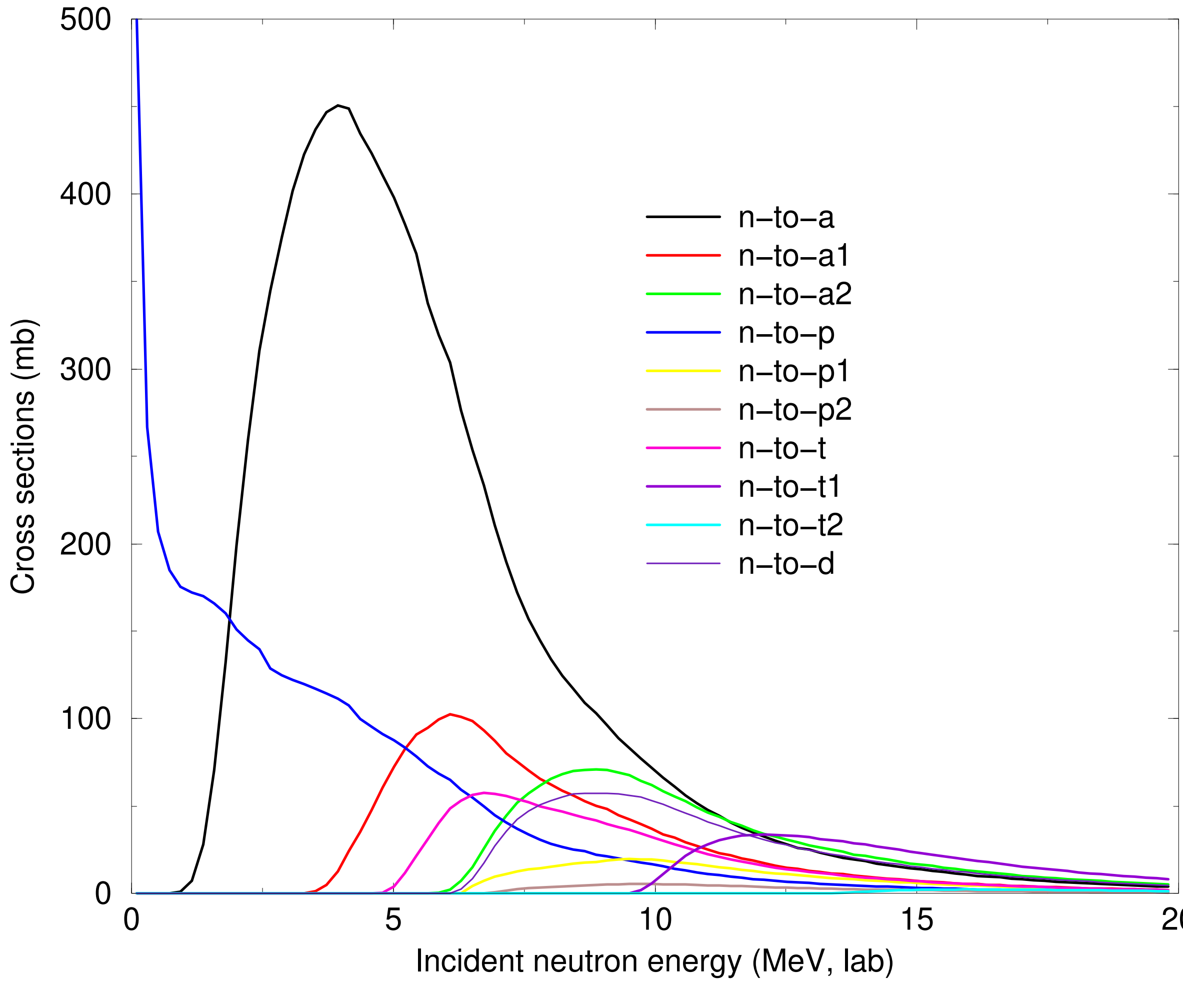
Hauser-Feshbach transfer cross-sections

Transfers

(n,a), (n,p), (n,t), (n,d)

Many larger than (n,n')

Fusion neutrons at 14 MeV will require all these transfer channels and more !

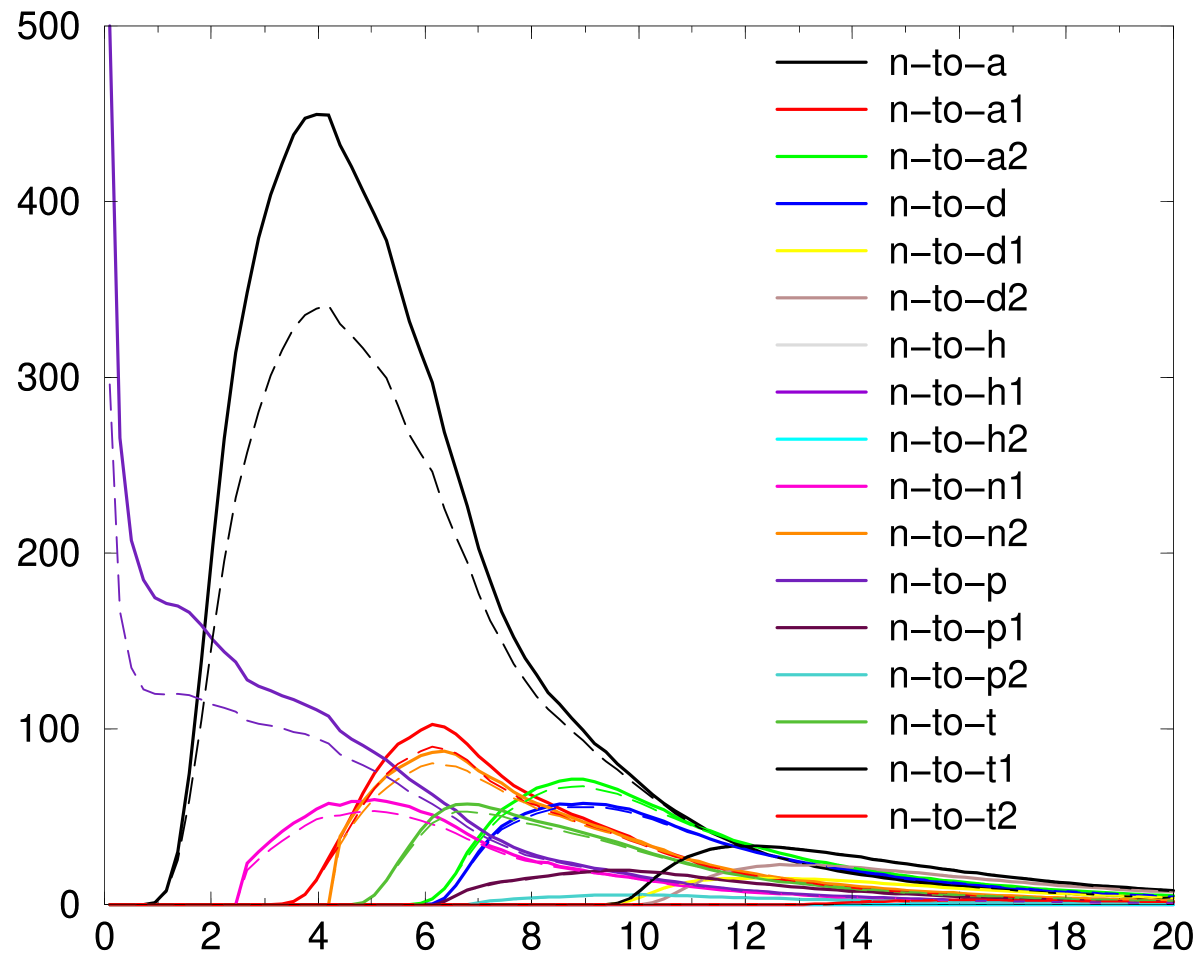


Hauser-Feshbach width-fluctuation corrections

Dashed lines use WFC from Moldauer PRC (1976), NPA (1980).

For neutrons, usually supposed to be small above 1 MeV, but here we see effects up to 9 MeV.

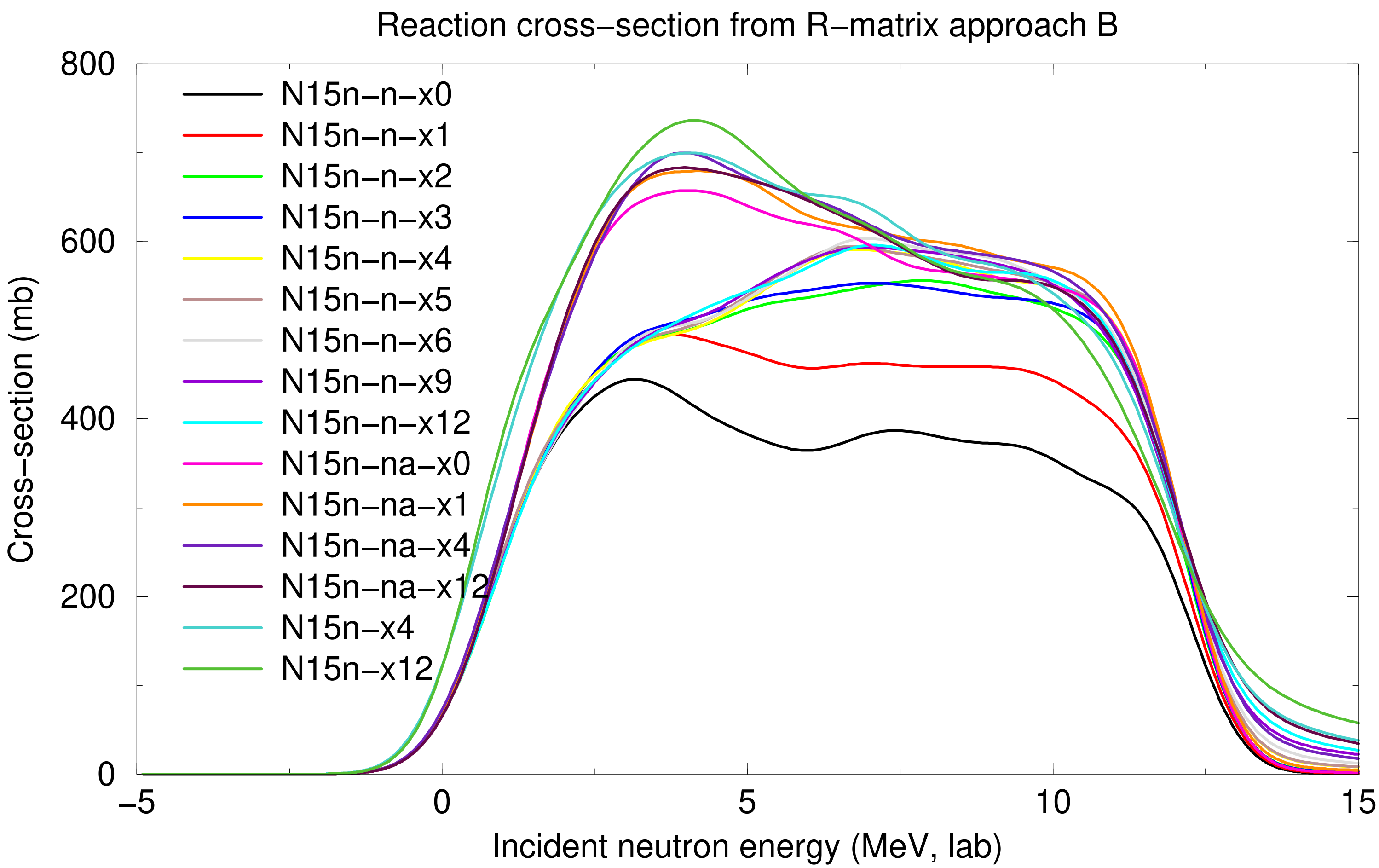
Use WFC calculated factor in YAHFC



Generate R-matrix poles from optical potential and level densities

- Start from optical potential for projectiles n, p, α (etc)
- Choose which nuclear excited states to include (x1, x4, … , x12)
- Use a level-density to generate spacings D up to 12 MeV.
- Find partial widths by A: $\langle \Gamma_\alpha \rangle = -\frac{D}{2\pi} \ln(|\mathbf{S}^{\text{opt}}_{\alpha\alpha}|^2)$
- Or by method B:: $\langle \Gamma_\alpha \rangle = \frac{D}{2\pi}(1 - |\mathbf{S}^{\text{opt}}_{\alpha\alpha}|^2)$
- Or Ap, Bp: reduced width *amplitudes* have gaussian fluctuations
- Generate discrete levels with above statistics (like Dicebox)
- Find exact cross-sections from R-matrix theory
- Compare with HF results after smoothing (e.g. 1 MeV Gaussian)

Reaction cross-sections from R-matrix method B



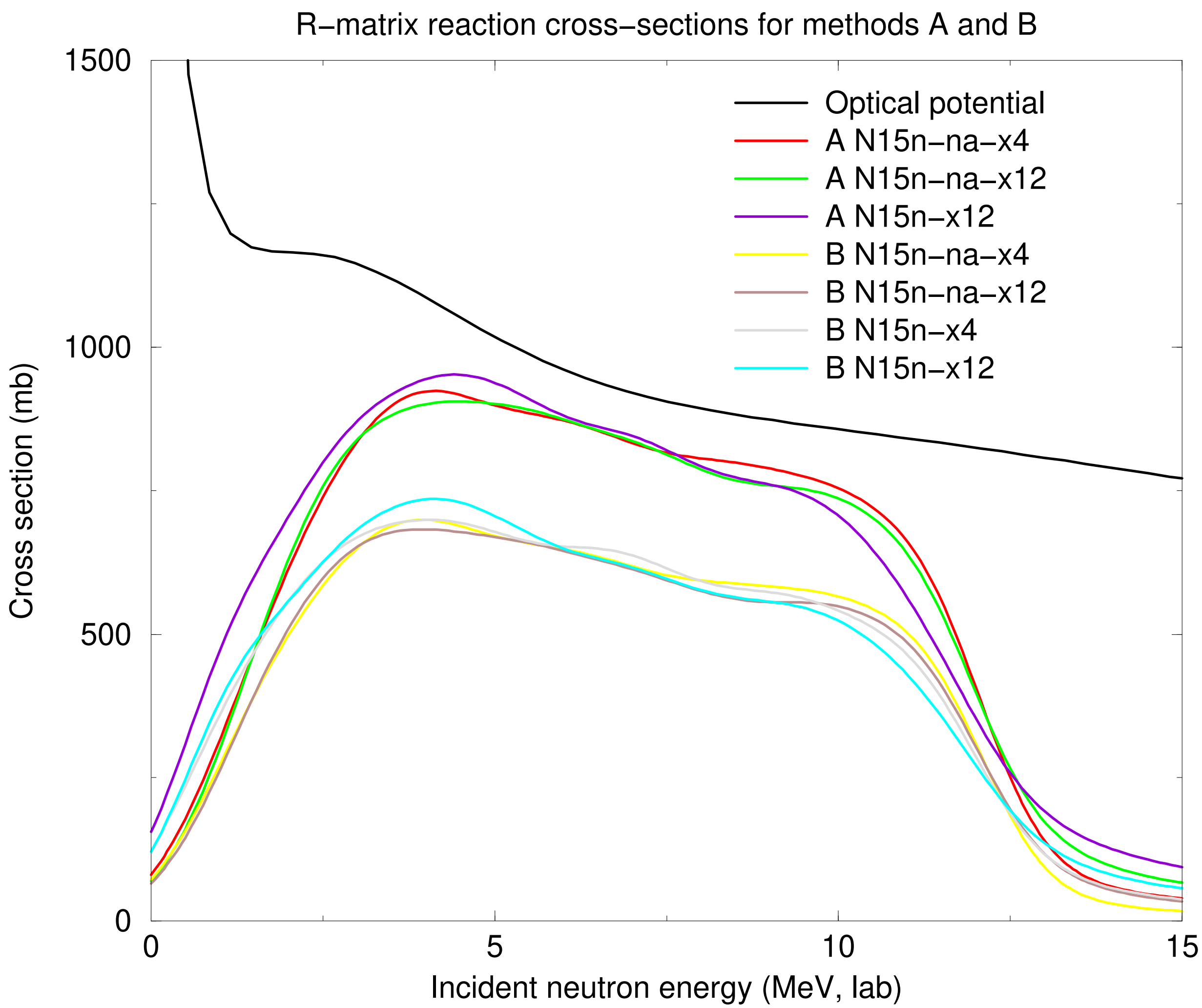
N15n-x is
n + α + p + d + t

Curves larger as more excited levels included.

Seems to converge

R-matrix poles only to 12 MeV

Comparing width methods A and B



R-matrix A method: γ magnitude normal N(0,mean): Porter-T.

R-matrix B method: γ magnitude fixed to mean, sign random

Method A gives reaction cross section nearest to that of the optical potential.

But strange short-coming at low energies.
May be compound-elastic.

R-matrix poles only to 12 MeV

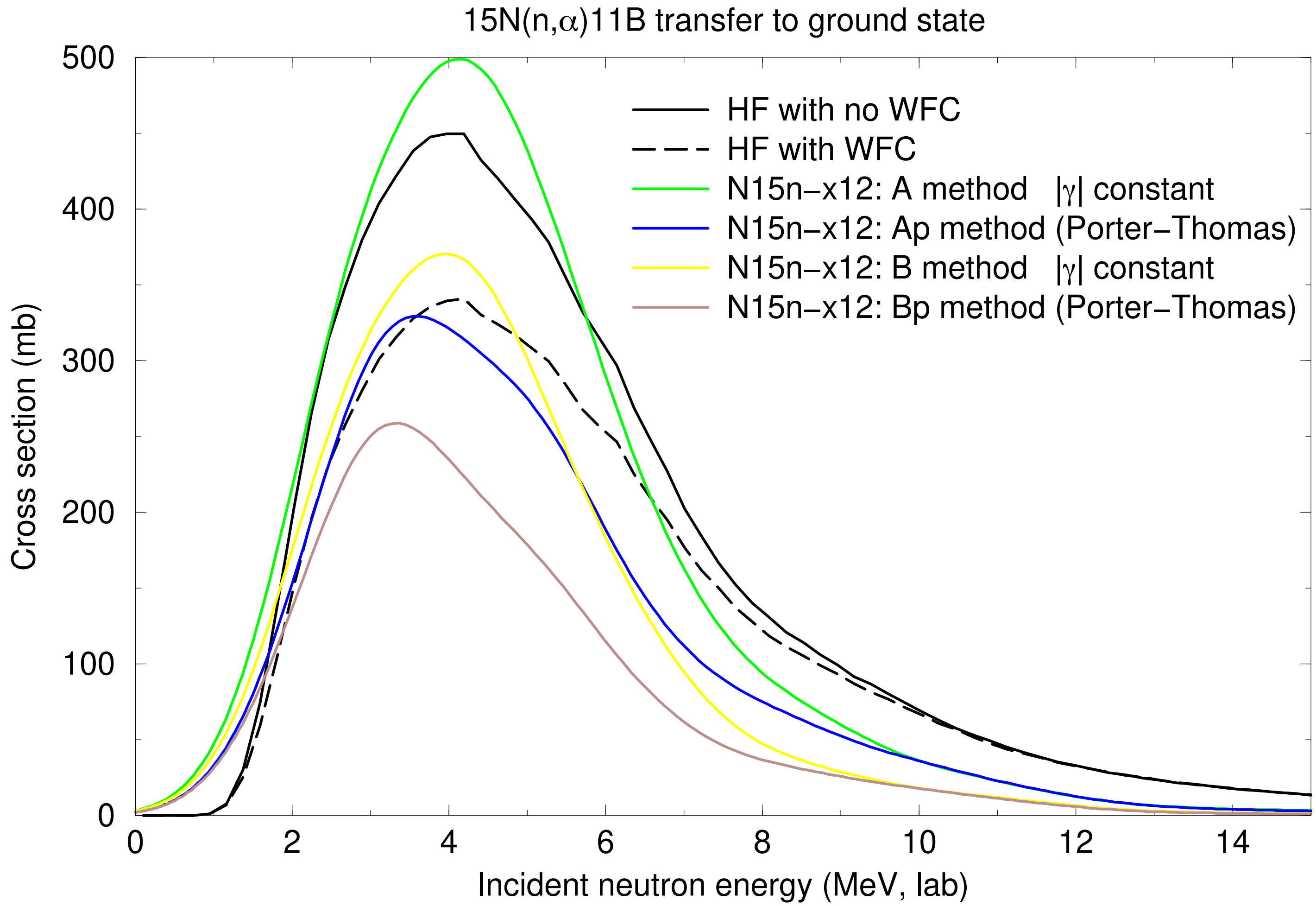
Channel Comparisons: HF and full R-matrix (A,B) - (n,α) channel

Most accurate are expected to be HF+WFC and Ap methods.

These two (blue and black-dashed) agree the best, at least up to ~ 5 MeV.

R-matrix A method: γ magnitude normal N(0,mean): Porter-T.

R-matrix B method: γ magnitude fixed to mean, sign random

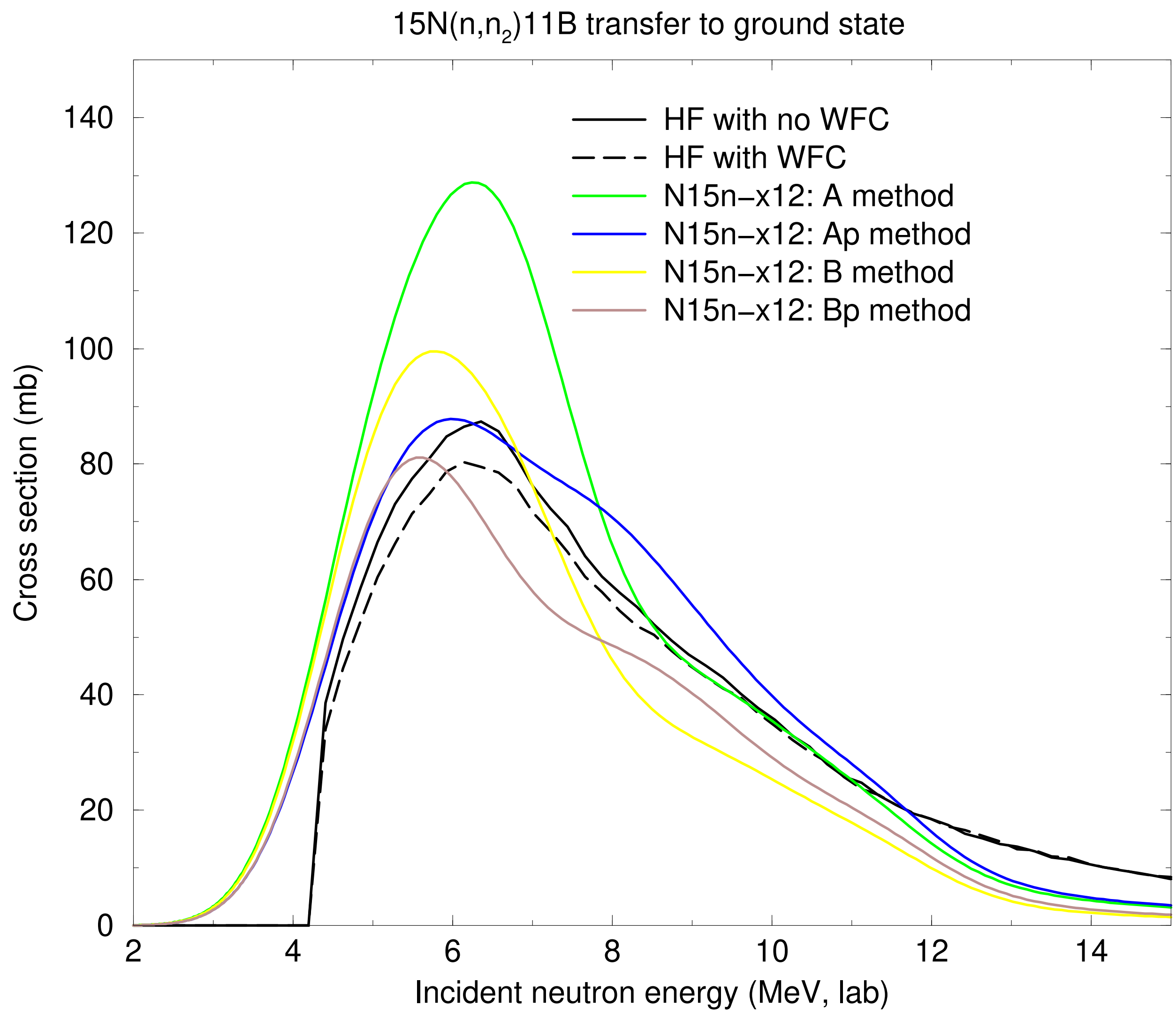


Channel Comparisons: HF and full R-matrix (A,B) - (n,n_2) channel

Most accurate are expected to be HF+WFC and Ap methods.

HF and Ap methods (blue and black) agree the best, at least up to ~ 7 MeV.

WFC does not have large effects here.



Summary

- Possible to compare full R-matrix and Hauser-Feshbach models in transition region of unresolved resonances
- Necessary to include all excited residual states up to incident energy. This is well-known for HF, but not so well for R-matrix. (Needed anyway to predict gamma production cross-sections)
- Makes large R-matrix model: I use tensorflow of GPUs.
- Demonstrate best comparison agreements when including
  - Width-fluctuation corrections in HF (up to higher energies)
  - Full Porter-Thomas statistics of reduced width amplitudes $\gamma_{p\alpha}$.
- These are well known for high-A targets, but here for N15 too.

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